

Nitroethane
79-24-3 | DTXSID8020969

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: -89.2 °C

Global applicability domain: Inside

Local applicability domain index: 5.88e-01

Confidence level: 6.83e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Nitroethane</div> <div>Measured: -89.5</div> <div>Predicted: -89.2</div>	<div>Image not found</div> <div>n-Propyl nitrate</div> <div>Measured: -100</div> <div>Predicted: -98.6</div>	<div>Image not found</div> <div>Ethene, nitro-</div> <div>Measured: -55.5</div> <div>Predicted: -62.1</div>
<div>Image not found</div> <div>1-Nitropropane</div> <div>Measured: -108</div> <div>Predicted: -87.7</div>	<div>Image not found</div> <div>2-Nitropropane</div> <div>Measured: -91.3</div> <div>Predicted: -84.6</div>	